

# Implementation of Nano-scale Rectifiers: An Exact Study

Santanu K. Maiti<sup>1,2</sup>

<sup>1</sup>*Theoretical Condensed Matter Physics Division,*

*Saha Institute of Nuclear Physics, 1/AF, Bidhannagar, Kolkata-700 064, India*

<sup>2</sup>*Department of Physics, Narasinha Dutt College, 129 Belilious Road, Howrah-711 101, India*

We propose the possibilities of designing nano-scale rectifiers using mesoscopic rings. A single mesoscopic ring is used for half-wave rectification, while full-wave rectification is achieved using two such rings and in both cases each ring is threaded by a time varying magnetic flux  $\phi$  which plays a central role in the rectification action. Within a tight-binding framework, all the calculations are done based on the Green's function formalism. We present numerical results for the two-terminal conductance and current which support the general features of half-wave and full-wave rectifications. The analysis may be helpful in fabricating mesoscopic or nano-scale rectifiers.

PACS numbers: 73.63.-b, 73.63.Rt, 81.07.Nb

## I. INTRODUCTION

Low-dimensional model quantum systems have been the objects of intense research in theory as well as in experiment since these simple looking systems are prospective candidates for future generation of nano-devices in electronic engineering. Several striking features are exhibited by these systems owing to the quantum interference effect which is generally preserved throughout the sample only for much smaller sizes, while the effect disappears for larger systems. A normal metal mesoscopic ring is a very nice example where the electronic motion is confined and the transport becomes coherent. Current trend of miniaturization of electronic devices has resulted much interest in characterization of ring type nanostructures. There are several methods for preparation of such rings. For example, gold rings can be designed by using templates of suitable structure in combination with metal deposition via ion beam etching [1, 2]. More recently, Yan *et al.* have prepared gold rings by selective wetting of porous templates using polymer membranes [3]. Using such rings we can design nano-scale rectifiers and to reveal this fact the ring is coupled to two electrodes, to form an electrode-ring-electrode bridge, where AC signal is applied. Electron transport through a bridge system was first studied theoretically by Aviram and Ratner [4] in 1974. Following this pioneering work, several experiments have been done through different bridge systems to reveal the actual mechanism of electron transport. Though, to date a lot of theoretical [5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16] as well as experimental works [17, 18, 19, 20] on two-terminal electron transport have been done addressing several important issues, yet the complete knowledge of conduction mechanism in nano-scale systems is still unclear to us. Transport properties are characterized by several significant factors like quantization of energy levels, quantum interference of electronic waves associated with the geometry of bridging system adopts within the junction, etc. Electronic transport through a mesoscopic ring is highly sensitive on ring-to-electrode interface geometry. Chang-

ing the interface structure, transmission probability of an electron across the ring can be controlled efficiently. Furthermore, electron transport in the ring can also be modulated in other way by tuning the magnetic flux, the so-called Aharonov-Bohm (AB) flux, penetrated by the ring. The AB flux can change the phases of electronic wave functions propagating through different arms of the ring leading to constructive or destructive interferences, and accordingly, the transmission amplitude changes.

In the present work we illustrate the possibilities of designing nano-scale rectifiers using mesoscopic rings. To design a half-wave rectifier we use a single mesoscopic ring, while two such rings are considered for designing a full-wave rectifier. Both for the cases of half-wave and full-wave rectifiers, each ring is threaded by a time varying magnetic flux  $\phi$  which plays the central role for the rectification action. Within a tight-binding framework, a simple parametric approach [21, 22, 23, 24, 25, 26, 27, 28, 29] is given and all the calculations are done through single particle Green's function technique to reveal the electron transport. Here we present numerical results for the two-terminal conductance and current which clearly describe the conventional features of half-wave and full-wave rectifications. Our exact analysis may be helpful for designing mesoscopic or nano-scale rectifiers. To the best of our knowledge the rectification action using such simple mesoscopic rings has not been addressed earlier in the literature.

The paper is organized as follows. With the brief introduction (Section I), in Section II, we describe the model and the theoretical formulations for our calculations. Section III presents the significant results, and finally, we conclude our results in Section IV.

## II. MODEL AND SYNOPSIS OF THE THEORETICAL BACKGROUND

### A. Circuit configuration of a half-wave rectifier

We begin by referring to Fig. 1. A mesoscopic ring, threaded by a time varying magnetic flux  $\phi$ , is attached

symmetrically to two semi-infinite one-dimensional (1D) metallic electrodes, namely, source and drain. Two end points C and D of secondary winding of the transformer are directly coupled to the source and drain, respectively,

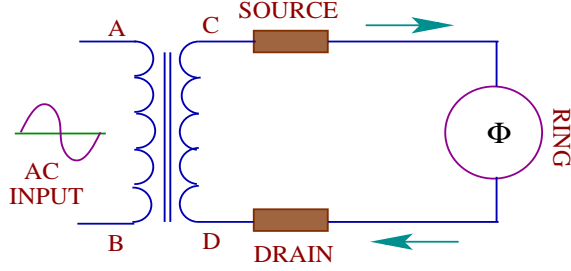


FIG. 1: (Color online). Circuit configuration for a half-wave rectifier, where a mesoscopic ring, subject to a time varying magnetic flux  $\phi$ , is attached symmetrically to source and drain. These electrodes are directly coupled to the end points C and D of secondary winding of the transformer. The arrow indicates current direction in the circuit.

through which AC signal is applied. Mathematically, we can express the AC signal in the form,

$$V(t) = V_0 \sin(\omega t) \quad (1)$$

where,  $V_0$  is the peak voltage,  $\omega$  corresponds to the angular frequency and  $t$  represents the time. For the rectification action, we choose the flux passing through the ring

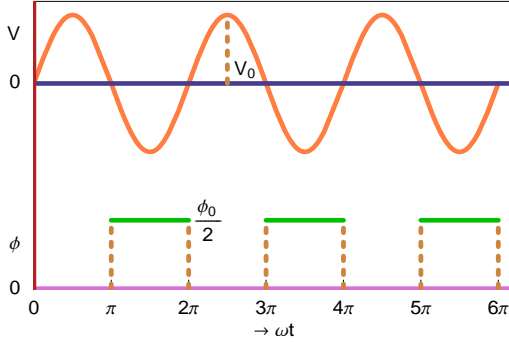


FIG. 2: (Color online). Variations of AC input signal (orange line) and magnetic flux (green line) as a function of time  $t$ .

in the square wave form as a function of time. Mathematically it can be written as,

$$\begin{aligned} \phi(t) &= 0 & \text{for } n\pi < \omega t < (n+1)\pi \\ & & \text{where, } n = 0 \text{ or any even integer} \\ &= \frac{\phi_0}{2} & \text{for } n\pi < \omega t < (n+1)\pi \\ & & \text{where, } n = \text{any odd integer} \end{aligned} \quad (2)$$

where,  $\phi_0 (= ch/e)$  is the elementary flux-quantum. Both the AC signal and threaded magnetic flux  $\phi$  vary periodically with the same frequency  $\omega$ . The variations of AC input signal (orange line) and magnetic flux (green line)

are represented graphically in Fig. 2. From the spectra it is clear that in the negative half-cycles of the input signal, the ring is penetrated by the flux  $\phi_0/2$ , which is required for half-wave rectification.

## B. Circuit configuration of a full-wave rectifier

The circuit diagram for a full-wave rectifier is schematically presented in Fig. 3. Here two mesoscopic rings are used, together with a transformer whose secondary winding is split equally into two and has a common center

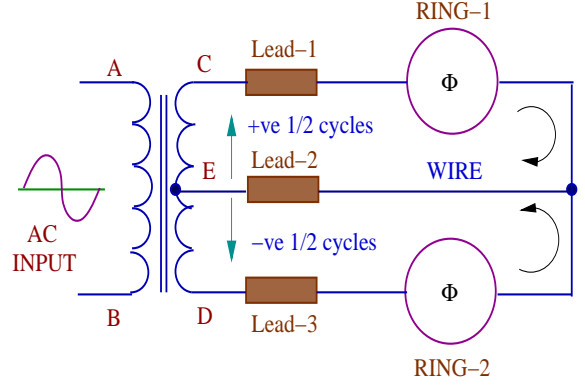


FIG. 3: (Color online). Circuit configuration for a full-wave rectifier using two mesoscopic rings, where each ring is threaded by a time varying magnetic flux. The arrows indicate current directions in the circuit.

tapped connection, described by the point E. The rings are threaded by time varying magnetic fluxes  $\phi_1$  and  $\phi_2$ , respectively, and their functional forms are described by

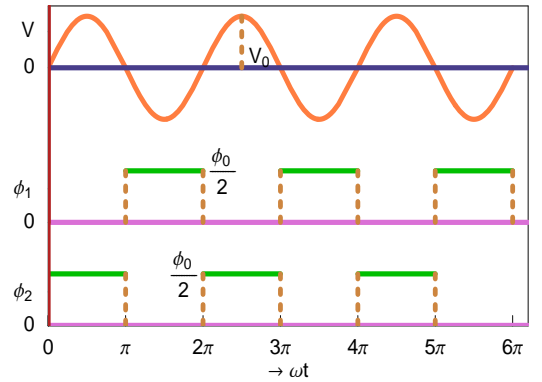


FIG. 4: (Color online). Variations of AC input voltage (orange curve) and magnetic fluxes (green curves) as a function of time  $t$ . A constant  $\pi$  phase shift exists between the fluxes,  $\phi_1$  and  $\phi_2$ , threaded by the rings.

Eq. 2. A constant  $\pi$  phase shift exists between these two fluxes, as schematically shown in Fig. 4, which is essential for full-wave rectification. In the circuit there are three electrodes, namely, lead-1, lead-2 and lead-3, those are directly coupled to the points C, E and D of secondary

winding of the transformer, respectively. During positive half-cycle of the AC input signal, lead-1 and lead-2 act as source and drain, respectively. While, for the negative half-cycle of the AC input voltage, lead-3 and lead-2 behave as source and drain, respectively. Thus the circuit consists of two half-wave rectifiers, as shown clearly from Fig. 3. Each rectifier is connected to a single quantum wire through which current flows in one direction during each half-cycle of the AC input signal which is described by the arrows in Fig. 3. The variations of AC input voltage (orange curve) and associated magnetic fluxes (green curves) in the rings are represented graphically in Fig. 4. From the spectra it is observed that, in the positive half-cycles of AC input signal, ring-2 is threaded by the flux  $\phi_0/2$ . On the other hand, for the negative half-cycles of the input signal, ring-1 is penetrated by the flux  $\phi_0/2$ .

### C. Theoretical formulation

Using Landauer conductance formula [30, 31] we determine two-terminal conductance ( $g$ ) of the mesoscopic ring. At much low temperatures and bias voltage it ( $g$ ) can be written in the form,

$$g = \frac{2e^2}{h} T \quad (3)$$

where,  $T$  corresponds to the transmission probability of an electron across the ring. In terms of the Green's function of the ring and its coupling to two electrodes, the transmission probability can be expressed as [30, 31],

$$T = \text{Tr} [\Gamma_1 G_R^r \Gamma_2 G_R^a] \quad (4)$$

where,  $\Gamma_S$  and  $\Gamma_D$  describe the coupling of the ring to the source and drain, respectively. Here,  $G_R^r$  and  $G_R^a$  are the retarded and advanced Green's functions, respectively, of the ring considering the effects of the electrodes. Now, for the full system i.e., the mesoscopic ring, source and drain, the Green's function is expressed as,

$$G = (E - H)^{-1} \quad (5)$$

where,  $E$  is the energy of the source electron. Evaluation of this Green's function needs the inversion of an infinite matrix, which is really a difficult task, since the full system consists of the finite size ring and two semi-infinite 1D electrodes. However, the full system can be partitioned into sub-matrices corresponding to the individual sub-systems and the effective Green's function for the ring can be written in the form [30, 31],

$$G_R = (E - H_R - \Sigma_S - \Sigma_D)^{-1} \quad (6)$$

where,  $H_R$  describes the Hamiltonian of the ring. Within the non-interacting picture, the tight-binding Hamilto-

nian of the ring can be expressed like,

$$H_R = \sum_i \epsilon_i c_i^\dagger c_i + \sum_{\langle ij \rangle} v \left( c_i^\dagger c_j e^{i\theta} + c_j^\dagger c_i e^{-i\theta} \right) \quad (7)$$

where,  $\epsilon_i$  and  $v$  correspond to the site energy and nearest-neighbor hopping strength, respectively.  $c_i^\dagger$  ( $c_i$ ) is the creation (annihilation) operator of an electron at the site  $i$  and  $\theta = 2\pi\phi/N\phi_0$  is the phase factor due to the flux  $\phi$  enclosed by the ring consists of  $N$  atomic sites. A similar kind of tight-binding Hamiltonian is also used, except the phase factor  $\theta$ , to describe the electrodes where the Hamiltonian is parametrized by constant on-site potential  $\epsilon'$  and nearest-neighbor hopping integral  $t'$ . The hopping integral between the ring and source is  $\tau_S$ , while it is  $\tau_D$  between the ring and drain. In Eq. (6),  $\Sigma_S$  and  $\Sigma_D$  are the self-energies due to the coupling of the ring to the source and drain, respectively, where all the information of the coupling are included into these self-energies.

To determine current, passing through the mesoscopic ring, we use the expression [30, 31],

$$I(V) = \frac{2e}{h} \int_{-\infty}^{\infty} (f_S - f_D) T(E) dE \quad (8)$$

where,  $f_{S(D)} = f(E - \mu_{S(D)})$  gives the Fermi distribution function with the electrochemical potential  $\mu_{S(D)} = E_F \pm eV/2$  and  $E_F$  is the equilibrium Fermi energy. For the sake of simplicity, we take the unit  $e = h = 1$  in our present calculations.

## III. NUMERICAL RESULTS AND DISCUSSION

To illustrate the results, let us begin our discussion by mentioning the values of different parameters used for our numerical calculations. In the mesoscopic ring, the on-site energy  $\epsilon_i$  is fixed to 0 for all the atomic sites  $i$  and nearest-neighbor hopping strength  $v$  is set to 3. While, for the side-attached electrodes the on-site energy ( $\epsilon'$ ) and nearest-neighbor hopping strength ( $t'$ ) are chosen as 0 and 4, respectively. The hopping strengths  $\tau_S$  and  $\tau_D$  are set as  $\tau_S = \tau_D = 2.5$ . The equilibrium Fermi energy  $E_F$  is taken as 0.

### A. Half-wave rectification

The rectification action of the half-wave rectifier is illustrated in Fig. 5. In the upper panel of this figure we plot AC input signal (orange curve) as a function of  $\omega t$ . The amplitude  $V_0$  of the AC signal is fixed at 2. The variation of conductance  $g$  (red curve) as a function of  $\omega t$  is shown in the middle panel. From the results we clearly observe that only in the positive half-cycles of the AC input signal, conductance exhibits finite value. On the other hand, conductance exactly drops to zero for

the negative half-cycles of the AC input signal.  $g_{max}$  is the amplitude of the conductance which gets the value 2, and therefore, the transmission probability  $T$  goes to unity, according to Landauer conductance formula (see Eq. 3). Now we try to figure out the rectification operation. The probability amplitude of getting an electron from the source to drain across the ring depends on the quantum interference effect of the electronic waves passing through the upper and lower arms of the ring. For a symmetrically connected ring (upper and lower arms are identical to each other), threaded by a magnetic flux  $\phi$ , the probability amplitude of getting an electron across the ring becomes exactly zero ( $T = 0$ ) for the typical flux,  $\phi = \phi_0/2$ . This vanishing behavior of the transmission probability can be easily obtained through few simple mathematical steps. Therefore, in the negative half cycles of the AC input signal, electron conduction through the ring is no longer possible since the ring encloses the flux  $\phi_0/2$  for these half-cycles. Only for the

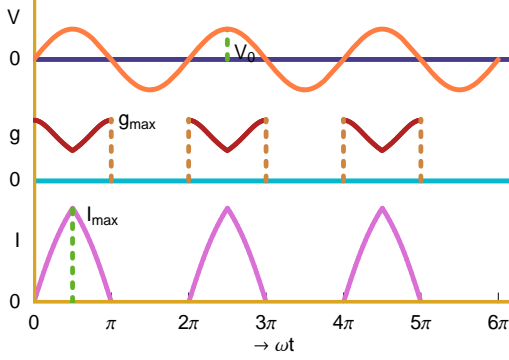


FIG. 5: (Color online). Half-wave rectification action. Upper panel describes AC input signal of amplitude  $V_0$ . Middle panel illustrates the variation of conductance  $g$  with  $\omega t$ . Lower panel represents the variation of current  $I$  as a function of  $\omega t$ .  $g_{max}$  and  $I_{max}$  correspond to the conductance and current maxima, respectively. Here we set the ring size  $N = 8$ .

positive half-cycles of the AC input signal electron can conduct through the ring as the ring is not penetrated by the flux  $\phi_0/2$ . This feature clearly describes the half-wave rectification action. To visualize the rectification feature more prominently we present the variation of current (magenta curve) as a function of  $\omega t$  in the lower panel of Fig. 5. We obtain the current  $I$  through the ring by integrating over the transmission function  $T$  (see Eq. 8). Following the conductance pattern (red curve), the vanishing nature of the current in the negative half-cycles of the AC input signal is clearly understood. The non-vanishing behavior (magenta curve) of the current is only achieved for the positive half-cycles of the AC input. All these features clearly support the half-wave rectification action as we get in traditional macroscopic half-wave rectifiers.

## B. Full-wave rectification

Next, we investigate the behavior of full-wave rectification mechanism as illustrated in Fig. 6. The upper, middle and lower panels correspond to the time varying features of input signal, conductance and current, respectively. Our results demonstrate that both for the positive and negative half-cycles of the input signal non-zero conductance (red curve) is obtained. During the positive half-cycles ring-1 conducts, while for the negative half-cycles conduction takes place through ring-2, as both the two rings enclose time varying magnetic fluxes having identical magnitude  $\phi_0/2$  with a constant phase shift  $\pi$ . The feature of full-wave rectification i.e., obtaining

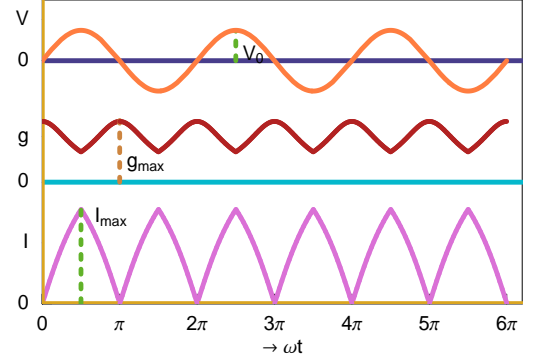


FIG. 6: (Color online). Full-wave rectification action. Upper panel describes AC input signal of amplitude  $V_0$ . Middle panel illustrates the variation of conductance  $g$  with  $\omega t$ . Lower panel represents the variation of current  $I$  as a function of  $\omega t$ .  $g_{max}$  and  $I_{max}$  correspond to the conductance and current maxima, respectively. Here we fix the ring size  $N = 8$ .

non-zero conductance for both positive and negative half-cycles of the input signal is attributed to the quantum interference effect as explained earlier in case of half-wave rectification. In the same footing, here we describe the variation of current  $I$  (magenta curve) with time  $t$  to support the full-wave rectification operation properly. Here also non-zero value of current is achieved both for the positive and negative half-cycles of the input signal following the conductance spectrum. Our results support the full-wave rectification action and agree well with the basic features obtained in conventional macroscopic full-wave rectifiers.

## IV. CONCLUDING REMARKS

In a nutshell, we have proposed the possibilities of designing nano-scale rectifiers using mesoscopic rings enclosing a time varying magnetic flux. The half-wave rectifier is designed using a single mesoscopic rings, while two such rings are used for full-wave rectification. The rectification action is achieved using the central idea of quantum interference effect in presence of flux  $\phi$  in ring shaped geometries. We adopt a simple tight-binding framework

to illustrate the model and all the calculations are done using single particle Green's function formalism. Our exact numerical results provide two-terminal conductance and current which support the general features of half-wave and full-wave rectifications. Our analysis can be used in designing tailor made nano-scale rectifiers.

Throughout our work, we have addressed all the essential features of rectification operation considering a ring with total number of atomic sites  $N = 8$ . In our model calculations, this typical number ( $N = 8$ ) is chosen only for the sake of simplicity. Though the results presented here change numerically with the ring size ( $N$ ), but all the basic features remain exactly invariant. To be more specific, it is important to note that, in real situation the experimentally achievable rings have typical diameters within the range 0.4-0.6  $\mu\text{m}$ . In such a small ring, unrealistically very high magnetic fields are required to

produce a quantum flux. To overcome this situation, Hod *et al.* have studied extensively and proposed how to construct nanometer scale devices, based on Aharonov-Bohm interferometry, those can be operated in moderate magnetic fields [32, 33, 34, 35].

In the present paper we have done all the calculations by ignoring the effects of the temperature, electron-electron correlation, etc. Due to these factors, any scattering process that appears in the mesoscopic ring would have influence on electronic phases, and, in consequences can disturb the quantum interference effects. Here we have assumed that, in our sample all these effects are too small, and accordingly, we have neglected all these factors in this particular study.

The importance of this article is mainly concerned with (i) the simplicity of the geometry and (ii) the smallness of the size.

- 
- [1] K. L. Hobbs, P. R. Larson, G. D. Lian, J. C. Keay, and M. B. Johnson, *Nano Lett.* **4**, 167 (2004).
  - [2] D. H. Pearson, R. J. Tonucci, K. M. Bussmann, and E. A. Bolden, *Adv. Mater.* **11**, 769 (1999).
  - [3] F. Yan and W. A. Geodel, *Nano Lett.* **4**, 1193 (2004).
  - [4] A. Aviram and M. Ratner, *Chem. Phys. Lett.* **29**, 277 (1974).
  - [5] M. Magoga and C. Joachim, *Phys. Rev. B* **59**, 16011 (1999).
  - [6] J.-P. Launay and C. D. Coudret, in: A. Aviram and M. A. Ratner (Eds.), *Molecular Electronics*, New York Academy of Sciences, New York, (1998).
  - [7] R. Baer and D. Neuhauser, *Chem. Phys.* **281**, 353 (2002).
  - [8] R. Baer and D. Neuhauser, *J. Am. Chem. Soc.* **124**, 4200 (2002).
  - [9] D. Walter, D. Neuhauser, and R. Baer, *Chem. Phys.* **299**, 139 (2004).
  - [10] K. Tagami, L. Wang, and M. Tsukada, *Nano Lett.* **4**, 209 (2004).
  - [11] R. H. Goldsmith, M. R. Wasielewski, and M. A. Ratner, *J. Phys. Chem. B* **110**, 20258 (2006).
  - [12] W. Y. Cui, S. Z. Wu, G. Jin, X. Zhao, and Y. Q. Ma, *Eur. Phys. J. B* **59**, 47 (2007).
  - [13] P. A. Orellana, M. L. Ladrón de Guevara, M. Pacheco, and A. Latge, *Phys. Rev. B* **68**, 195321 (2003).
  - [14] P. A. Orellana, F. Dominguez-Adame, I. Gomez, and M. L. Ladrón de Guevara, *Phys. Rev. B* **67**, 085321 (2003).
  - [15] B. T. Pickup and P. W. Fowler, *Chem. Phys. Lett.* **459**, 198 (2008).
  - [16] P. Földi, B. Molnar, M. G. Benedict, and F. M. Peeters, *Phys. Rev. B* **71**, 033309 (2005).
  - [17] J. Chen, M. A. Reed, A. M. Rawlett, and J. M. Tour, *Science* **286**, 1550 (1999).
  - [18] M. A. Reed, C. Zhou, C. J. Muller, T. P. Burgin, and J. M. Tour, *Science* **278**, 252 (1997).
  - [19] T. Dadoosh, Y. Gordin, R. Krahne, I. Khivrich, D. Mahalu, V. Frydman, J. Sperling, A. Yacoby, and I. Bar-Joseph, *Nature* **436**, 677 (2005).
  - [20] C. M. Fischer, M. Burghard, S. Roth, and K. V. Klitzing, *Appl. Phys. Lett.* **66**, 3331 (1995).
  - [21] V. Mujica, M. Kemp, and M. A. Ratner, *J. Chem. Phys.* **101**, 6849 (1994).
  - [22] S. K. Maiti, *Solid State Commun.* **149**, 1684 (2009).
  - [23] V. Mujica, M. Kemp, A. E. Roitberg, and M. A. Ratner, *J. Chem. Phys.* **104**, 7296 (1996).
  - [24] S. K. Maiti, *Phys. Lett. A* **373**, 4470 (2009).
  - [25] M. P. Samanta, W. Tian, S. Datta, J. I. Henderson, and C. P. Kubiak, *Phys. Rev. B* **53**, R7626 (1996).
  - [26] S. K. Maiti, *J. Phys. Soc. Jpn.* **78**, 114602 (2009).
  - [27] M. Hjort and S. Stafström, *Phys. Rev. B* **62**, 5245 (2000).
  - [28] K. Walczak, *Cent. Eur. J. Chem.* **2**, 524 (2004).
  - [29] K. Walczak, *Phys. Stat. Sol. (b)* **241**, 2555 (2004).
  - [30] S. Datta, *Electronic transport in mesoscopic systems*, Cambridge University Press, Cambridge (1997).
  - [31] M. B. Nardelli, *Phys. Rev. B* **60**, 7828 (1999).
  - [32] O. Hod, R. Baer, and E. Rabani, *J. Phys. Chem. B* **108**, 14807 (2004).
  - [33] O. Hod, R. Baer, and E. Rabani, *J. Phys.: Condens. Matter* **20**, 383201 (2008).
  - [34] O. Hod, R. Baer, and E. Rabani, *J. Am. Chem. Soc.* **127**, 1648 (2005).
  - [35] O. Hod, E. Rabani, and R. Baer, *Acc. Chem. Res.* **39**, 109 (2006).